

PD; 00-00-00

### Substance

P: 1-2

Beilstein Registry Number 7581786

Chemical Name (3-decyloxy-propenyl)-benzene

Autoname (3-decyloxy-propenyl)-benzene

Molecular Formula C19H30O Molecular Weight 274.45 Lawson Number 5350, 362

Structure Keyword Stereo compound

Compound Type isocyclic Constitution ID 6430591 Tautomer ID 7109167 Beilstein Reference 6-06 Entry Date 1997/04/28 Update Date

### Reaction 1 of 2

Reaction ID 4557653

Reactant BRN 5616638 decan-1-ol; sodium salt

1098930 (3-bromo-1-propenyl)benzene

Product BRN 7581786 (3-decyloxy-propenyl)-benzene

1998/03/04

No. of Reaction Details

Reaction Classification Preparation

Reagent tetrabutylammonium iodide

6042944; Journal; Ochiai, Masahito; Ito, Takao; Takahushi, Hideo; Nakanishi, Akinobu; Ref. 1 Toyonari, Mika; et al.; JACSAT; J.Amer.Chem.Soc.; EN; 118; 33; 1996; 7716-7730;

## Reaction 2 of 2

Reaction ID 4585338

Reactant BRN 7581786 (3-decyloxy-propenyl)-benzene Product BRN 3203471 trans-cinnamic acid decyl ester

No. of Reaction Details

Reaction Classification Preparation

Yield 72 percent (BRN=3203471)

Reagent 1-(tert-butylperoxy)-1,2-benziodoxol-3(1H)-one, Cs2CO3

Solvent cyclohexane Time 51 hour(s) Temperature 25 C

6042944; Journal; Ochiai, Masahito; Ito, Takao; Takahushi, Hideo; Nakanishi, Akinobu; Ref. 1

# Nuclear Magnetic Resonance 1 of 2

Description Nucleus Solvents	Chemical shifts 1H CDCl3
Ref. 1	6042944; Journal; Ochiai, Masahito; Ito, Takao; Takahushi, Hideo; Nakanishi, Akinobu; Toyonari, Mika; et al.; JACSAT; J.Amer.Chem.Soc.; EN; 118; 33; 1996; 7716-7730;

# Nuclear Magnetic Resonance 2 of 2

Description Solvents	Spin-spin coupling constants CDCl3	
Note 1	1H-1H	
Ref. 1	6042944; Journal; Ochiai, Masahito; Ito, Takao; Takahushi, Hideo; Nakanishi, Akinobu; Toyonari, Mika; et al.; JACSAT; J.Amer.Chem.Soc.; EN; 118; 33; 1996; 7716-7730;	